

Parallel Adaptive Low Mach Number Simulation of Turbulent Combustion

John Bell

jb主bell@lbl.gov

Center for Computational Sciences and Engineering

Lawrence Berkeley National Laboratory, USA

<http://seesar.lbl.gov/ccse/>

Presented at: SciDAC 06
Denver, CO
June 25-29, 2006

Collaborators: M. Day, A. Almgren, M. Lijewski, C. Rendleman
R. K. Cheng, I. G. Shepherd

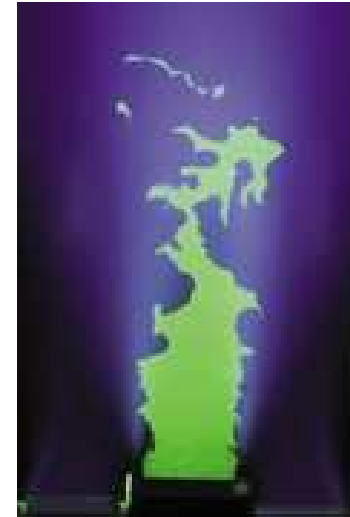
Lean Premixed Turbulent Combustion



Rod-stabilized V-flame



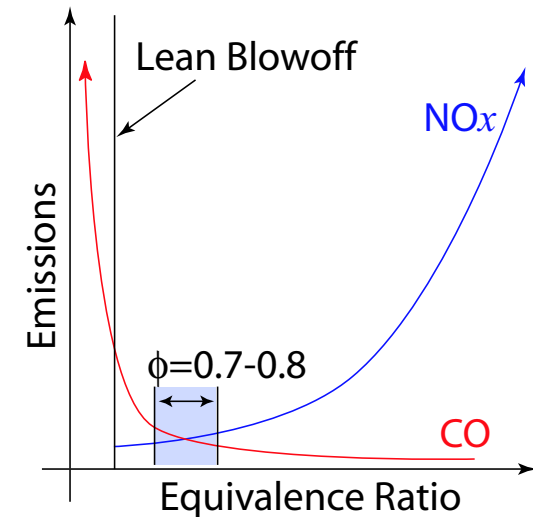
4-jet Low-swirl burner (LSB)



Slot burner

Study these types of flame computationally

- Potential for efficient, low-emission power systems
- Design issues because of flame instabilities
- Limitations of theory and experiment



Basic Physics of Combustion

Focus on gas phase combustion

Fluid mechanics

- Conservation of mass
- Conservation of momentum
- Conservation of energy

Thermodynamics

- Pressure, density, temperature relationships for multicomponent mixtures

Chemistry

- Reaction kinetics

Species transport

- Diffusive transport of different chemical species within the flame

Radiation

- Energy emission by hot gases

Low-swirl burner



- Operates in lean premixed combustion mode
- Ultra-low NO_x
- Interest in alternative fuels

Relevant Scales

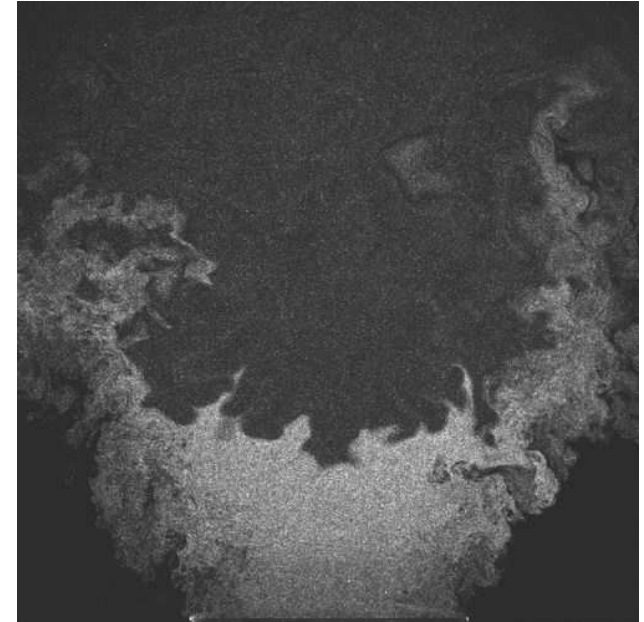
Spatial Scales

- Domain: ≈ 10 cm
- Flame thickness: $\delta_T \approx 1$ mm
- Integral scale: $\ell_t \approx 2 - 6$ mm

Temporal Scales

- Flame speed $O(10^2)$ cm/s
- Mean Flow: $O(10^3)$ cm/s
- Acoustic Speed: $O(10^5)$ cm / s

Fast chemical time scales but energy release coupling chemistry to fluid is on slower time scales



Mie Scattering Image

Simulation issues

- Wide range of length and time scale
- Multi-physics

Overview

Objective: Simulate turbulent premixed flames with:

1. No explicit model for turbulence, or turbulence/chemistry interactions
2. Detailed chemistry based on fundamental reactions, detailed diffusion
3. “Sufficient” range of scales to represent realistic flames

Traditional simulation approach essentially intractable

Exploit mathematical structure to compute more efficiently

Components of a computational model

- Mathematical model: describe the science in a way that is amenable to representation in a computer simulation
- Approximation / discretization: approximate the mathematical model with a finite number of degrees of freedom
- Solvers and software: develop algorithms for solving the discrete approximation efficiently on high-end architecture

Mathematical formulation

Exploit natural separation of scales between fluid motion and acoustic wave propagation

Low Mach number model, $M = U/c \ll 1$ (Rehm & Baum 1978, Majda & Sethian 1985)

Start with the compressible Navier-Stokes equations for multicomponent reacting flow, and expand in the Mach number, $M = U/c$.

Asymptotic analysis shows that:

$$p(\vec{x}, t) = p_0(t) + \pi(\vec{x}, t) \quad \text{where} \quad \pi/p_0 \sim \mathcal{O}(M^2)$$

- p_0 does not affect local dynamics, π does not affect thermodynamics
- For open containers p_0 is constant
- Pressure field is instantaneously equilibrated – removed acoustic wave propagation

Low Mach number equations

Momentum $\rho \frac{DU}{Dt} = -\nabla \pi + \nabla \cdot \left[\mu \left(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} - \frac{2}{3} \delta_{ij} \nabla \cdot U \right) \right]$

Species $\frac{\partial(\rho Y_m)}{\partial t} + \nabla \cdot (\rho U Y_m) = \nabla \cdot (\rho D_m \nabla Y_m) + \dot{\omega}_m$

Mass $\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho U) = 0$

Energy $\frac{\partial \rho h}{\partial t} + \nabla \cdot (\rho h \vec{U}) = \nabla \cdot (\lambda \nabla T) + \sum_m \nabla \cdot (\rho h_m D_m \nabla Y_m)$

Equation of state $p_0 = \rho \mathcal{R} T \sum_m \frac{Y_m}{W_m}$

System contains four evolution equations for U , Y_m , ρ , h , with a constraint given by the EOS.

Low Mach number system can be advanced at fluid time scale instead of acoustic time scale but . . .

We need effective integration techniques for this more complex formulation

Constraint for reacting flows

Low Mach number system is a system of PDE's evolving subject to a constraint; differential algebraic equation (DAE) with index 3

Differentiate constraint to reduce index

Here, we differentiate the EOS along particle paths and use the evolution equations for ρ and T to define a constraint on the velocity:

$$\begin{aligned}\nabla \cdot U &= \frac{1}{\rho} \frac{D\rho}{Dt} = -\frac{1}{T} \frac{DT}{Dt} - \frac{\mathcal{R}}{R} \sum_m \frac{1}{W_m} \frac{DY_m}{Dt} \\ &= \frac{1}{\rho c_p T} \left(\nabla \cdot (\lambda \nabla T) + \sum_m \rho D_m \nabla Y_m \cdot \nabla h_m \right) + \\ &\quad \frac{1}{\rho} \sum_m \frac{W}{W_m} \nabla (D_m \rho \nabla Y_m) + \frac{1}{\rho} \sum_m \left(\frac{W}{W_m} - \frac{h_m(T)}{c_p T} \right) \dot{\omega}_m \\ &\equiv S\end{aligned}$$

Incompressible Navier Stokes Equations



For iso-thermal, single fluid systems this analysis leads to the incompressible Navier Stokes equations

$$U_t + U \cdot \nabla U + \nabla \pi = \mu \Delta U$$

$$\nabla \cdot U = 0$$

How do we develop efficient integration schemes for this type of constrained evolution system?

Vector field decomposition

$$V = U_d + \nabla \phi$$

where $\nabla \cdot U_d = 0$

and

$$\int U \cdot \nabla \phi dx = 0$$

We can define a projection \mathbf{P}

$$\mathbf{P} = I - \nabla(\Delta^{-1})\nabla.$$

such that $U_d = \mathbf{P}V$

Solve

$$-\Delta \phi = \nabla \cdot V$$

Projection method

Incompressible Navier Stokes equations

$$U_t + U \cdot \nabla U + \nabla \pi = \mu \Delta U$$

$$\nabla \cdot U = 0$$

Projection method

Advection step

$$\frac{U^* - U^n}{\Delta t} + U \cdot \nabla U = 1/2 \mu \Delta (U^* + U_n) - \nabla \pi^{n-1/2}$$

Projection step

$$U^{n+1} = \mathbf{P} U^*$$

Recasts system as initial value problem

$$U_t + \mathbf{P}(U \cdot \nabla U - \mu \Delta U) = 0$$

How can this approach be generalized to low Mach number combustion?

- Finite amplitude density variations
- Compressibility effects

$$\frac{\partial U}{\partial t} + (U \cdot \nabla)U + \frac{1}{\rho} \nabla \pi = \frac{1}{\rho} \nabla \cdot \tau$$

$$\frac{\partial(\rho Y_m)}{\partial t} + \nabla \cdot (\rho U Y_m) = D_Y + R_Y$$

$$\frac{\partial(\rho h)}{\partial t} + \nabla \cdot (\rho U h) = D_h$$

$$\nabla \cdot U = S$$

Constant coefficient “projection”

- McMurtry, Riley, Metcalfe, AIAA J., 1986.
- Rutland & Fertziger, C&F, 1991.
- Zhang and Rutland, C&F, 1995.
- Cook and Riley, JCP, 1996.
- Najm, Trans. Phen. in Comb., 1996
- Najm & Wyckoff, C&F, 1997.
- Quian, Tryggvason & Law, JCP 1998.
- Najm, Knio & Wyckoff, JCP, 1998.

Variable coefficient projection

- Bell & Marcus, JCP, 1992.
- Lai, Bell, Colella, 11th AIAA CFD, 1993.
- Pember et al., Comb. Inst. WSS, 1995.
- Pember et al., Trans. Phen. Comb., 1996.
- Tomboulides et al., J. Sci. Comp., 1997.
- Pember et al., CST, 1998.
- Schneider et al., JCP, 1999.
- Day & Bell, CTM, 2000.
- Nicoud, JCP, 2000.

Variable coefficient projection

Generalized vector field decomposition

$$V = U_d + \frac{1}{\rho} \nabla \phi$$

where $\nabla \cdot U_d = 0$ and $U_d \cdot n = 0$ on the boundary

Then U_d and $\frac{1}{\rho} \nabla \phi$ are orthogonal in a density weighted space.

$$\int \frac{1}{\rho} \nabla \phi \cdot U \rho \, dx = 0$$

Defines a projection $\mathbf{P}_\rho = I - \frac{1}{\rho} \nabla ((\nabla \cdot \frac{1}{\rho} \nabla)^{-1}) \nabla \cdot$ such that $\mathbf{P}_\rho V = U_d$.

\mathbf{P}_ρ is idempotent and $\|\mathbf{P}_\rho\| = 1$

Generalized vector field decomposition

Use variable- ρ projection to define a generalized vector field decomposition

$$V = U_d + \nabla \xi + \frac{1}{\rho} \nabla \phi$$

where

$$\nabla \cdot \nabla \xi = S$$

and

$$\nabla \cdot U_d = 0$$

We can then define

$$U = \mathbf{P}_\rho(V - \nabla \xi) + \nabla \xi$$

so that $\nabla \cdot U = S$ with $\mathbf{P}_\rho(\frac{1}{\rho} \nabla \phi) = 0$

- This construct allows us to define a projection algorithm for variable density flows with inhomogeneous constraints
- Requires solution of a variable coefficient elliptic PDE
- Allows us to write system as a pure initial value problem

Low Mach number algorithm

Numerical approach based on generalized vector field decomposition

Fractional step scheme

- Advance velocity and thermodynamic variables
 - Advection
 - Diffusion
 - Stiff reactions
- Project solution back onto constraint

Stiff kinetics relative to fluid dynamical time scales

$$\frac{\partial(\rho Y_m)}{\partial t} + \nabla \cdot (\rho U Y_m) = \nabla \cdot (\rho D_m \nabla Y_m) + \dot{\omega}_m$$

$$\frac{\partial(\rho h)}{\partial t} + \nabla \cdot (\rho U h) = \nabla \cdot (\lambda \nabla T) + \sum_m \nabla \cdot (\rho h_m D_m \nabla Y_m)$$

Operator split approach

- Chemistry $\Rightarrow \Delta t/2$
- Advection – Diffusion $\Rightarrow \Delta t$
- Chemistry $\Rightarrow \Delta t/2$

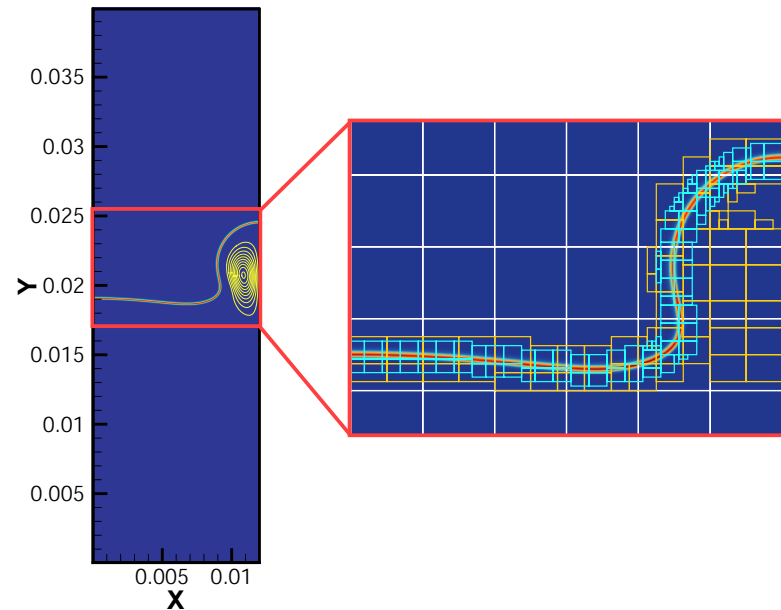
AMR – exploit varying resolution requirements in space and time

Block-structured hierarchical grids

- Amortize irregular work

Each grid patch (2D or 3D)

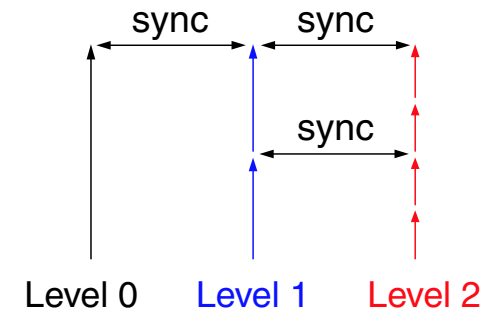
- Logically structured, rectangular
- Refined in space and time by evenly dividing coarse grid cells
- Dynamically created/destroyed



2D adaptive grid hierarchy

Subcycling:

- Advance level ℓ , then
 - Advance level $\ell + 1$
 - level ℓ supplies boundary data
 - Synchronize levels ℓ and $\ell + 1$



AMR Synchronization

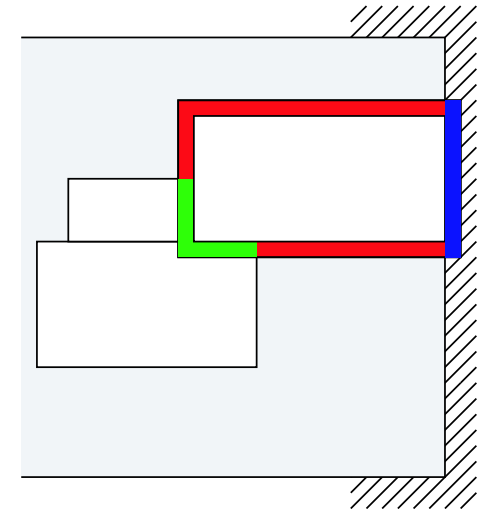
Coarse grid supplies Dirichlet data as boundary conditions for the fine grids.

Errors take the form of flux mismatches at the coarse/fine interface.

Design Principles:

- Define what is meant by the solution on the grid hierarchy.
- Identify the errors that result from solving the equations on each level of the hierarchy “independently”.
- Solve correction equation(s) to “fix” the solution.
- Correction equations match the structure of the process they are correcting.

- Fine-Fine
- Physical BC
- Coarse-Fine



Preserves properties of single-grid algorithm

Complex multiphysics application

- Advective transport – hyperbolic
- Diffusive transport – nonlinear parabolic systems
- Projections – variable coefficient elliptic equations
- Chemical kinetics – stiff ODE's

Dynamic adaptive refinement

Computation requires high-performance parallel architectures

Need to manage software complexity

- Develop data abstractions to support AMR algorithms
- Support parallelization strategy: Distribute grid patches to processors
- Encapsulate data / parallelization in reusable software framework

BoxLib foundation library:

- Domain specific class library: supports solution of PDE's on hierarchical structured adaptive grid
- Functionality for serial, distributed memory & shared memory parallel architectures
 - MPI communication
 - Programming interface through loop iteration constructs
 - Thread support for hierarchical parallelism

AMR framework library:

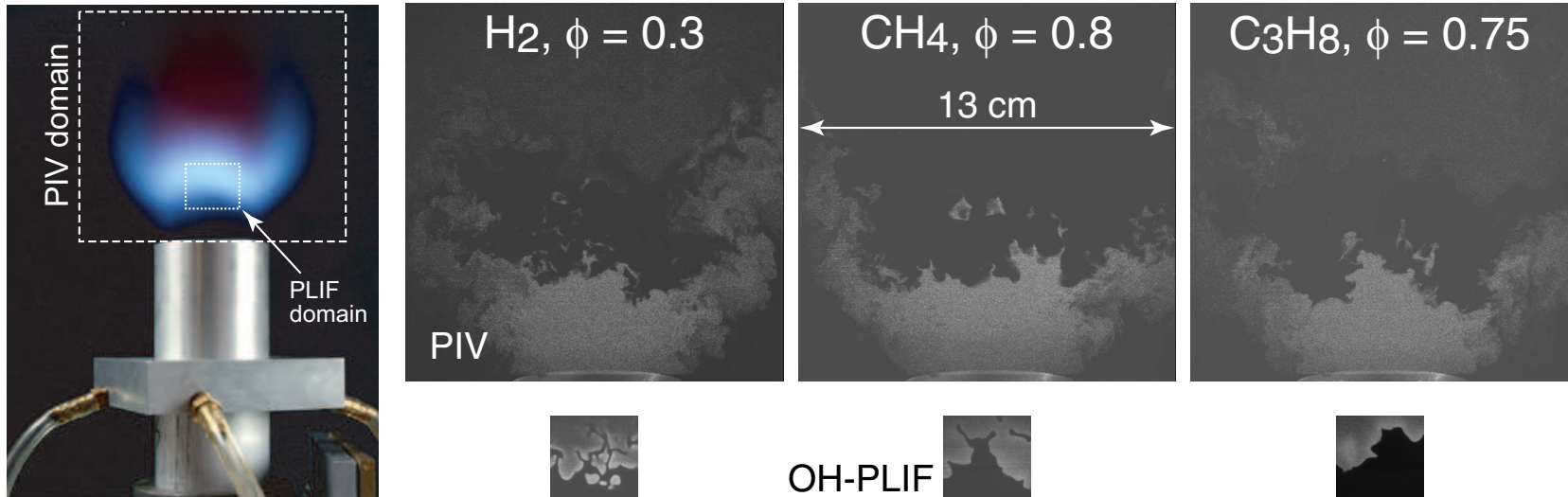
- Flow control, memory management, grid generation, checkpoint/restart and plotfile generation

Key issues in parallel implementation

- Dynamic load balancing
- Optimizing communication patterns
- Efficient manipulation of metadata
- Fast linear solvers

Combination of these computational elements make is possible to simulate realistic premixed turbulent flames

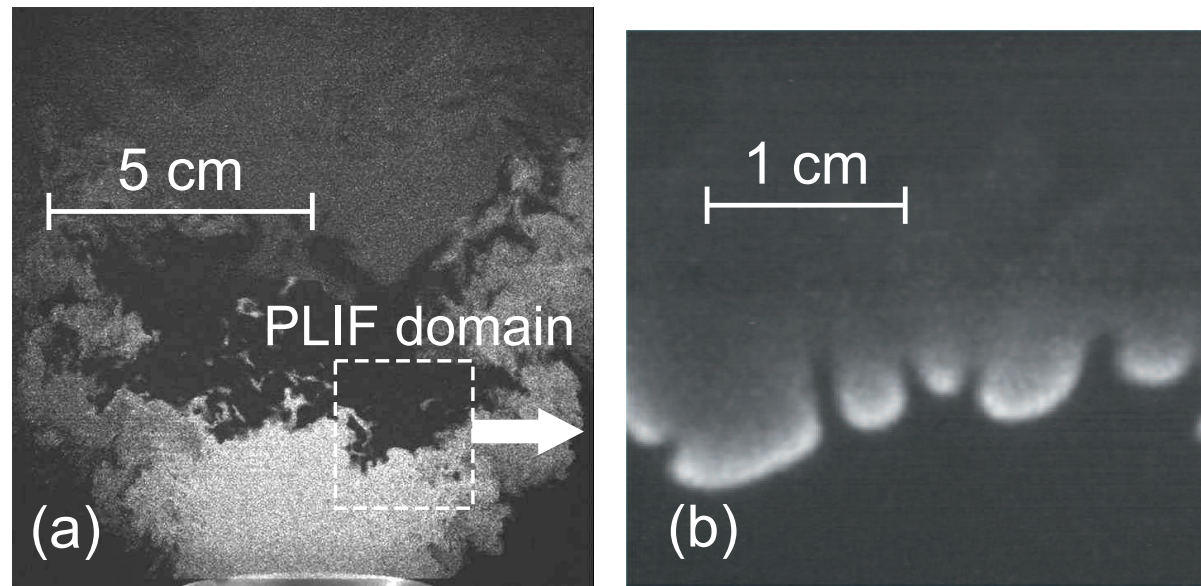
- Full-scale simulation of turbulent laboratory-scale flames
- Fuel effects in premixed combustion



Experiments focus on effect of different fuels on flame behavior

- Identical fueling rate/turbulence
- Nearly the same stabilization → nearly the same turbulent burning speed

Hydrogen combustion



- OH PLIF shows gaps in the flame
- Flame is not a continuous surface
- Standard flame analysis techniques not applicable

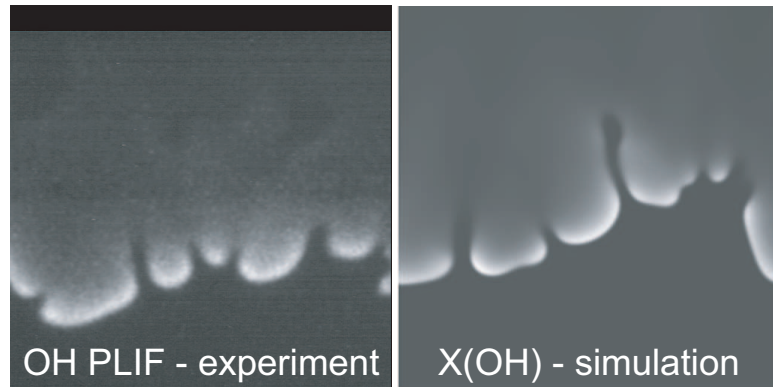
Use simulation to study ultra-lean premixed hydrogen flames

Focus on central core region

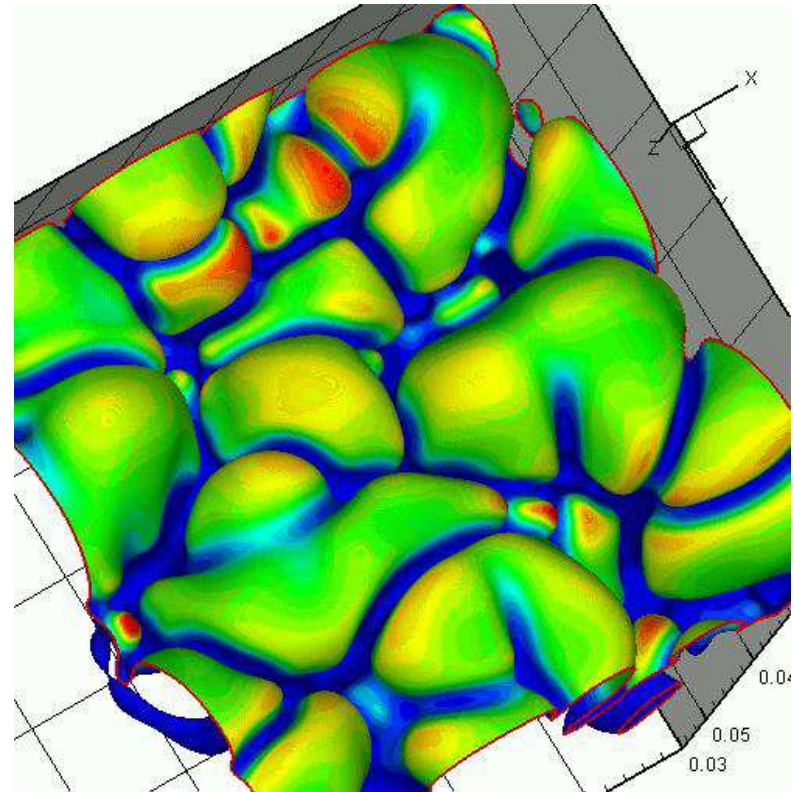
- Little swirl
- Weak net strain

Hydrogen flame in 3D

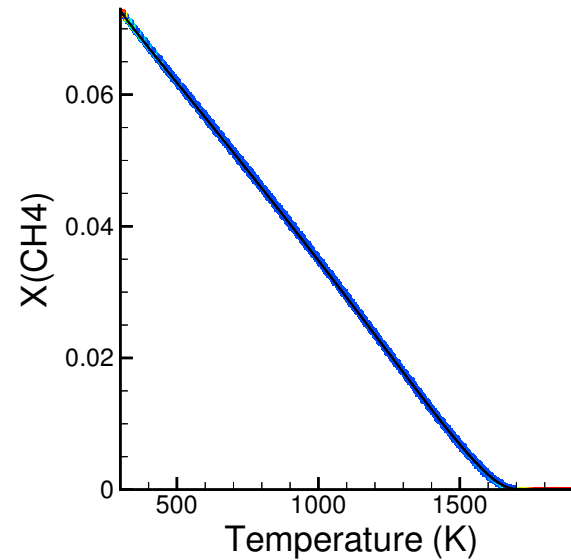
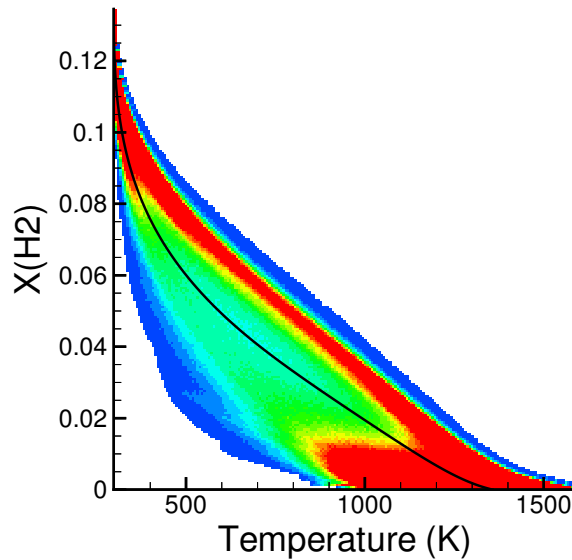
3D control simulation of detailed hydrogen flame at laboratory scales
($3 \times 3 \times 9$ cm domain, $\Delta x_f = 58 \mu\text{m}$)



- Figure is “underside” (from fuel side of flame)
- Flame surface (isotherm) colored by local fuel consumption
- Cellular structures convex to fuel, robust extinction ridges



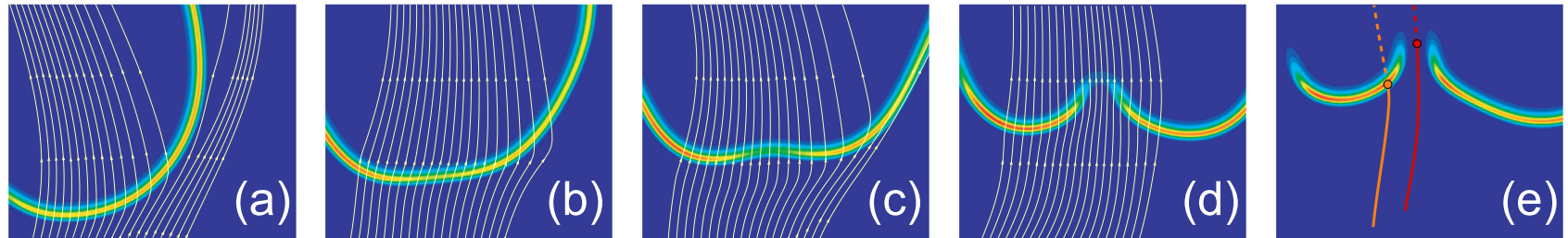
Chemistry in ultra-lean hydrogen flames



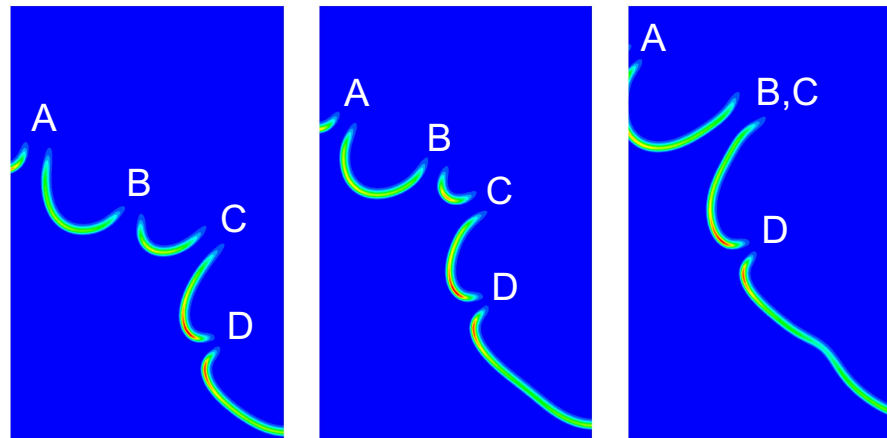
- Significant difference in burning characteristics
- Most burning occurs at conditions substantially different than laminar flame
- Burning occurs at richer conditions
- Fuel diffuses to burning region off of pathlines through extinction gaps

Localized hydrogen flame “extinction”

Analysis from 2D study



- Low-level localized strain event leads to onset of extinction.
- Lagrangian pathline analysis shows highly mobile fuel atoms diffuse “off-pathline”, no fuel leakage.



Extinction pockets once formed are very robust

Goal: Develop methodology to simulate realistic flames

- Range of scales relevant to laboratory experiments
- Detailed chemistry and transport
- No explicit models for turbulence or turbulence / chemistry interaction

Consider all aspects of the problem

- Low Mach number formulation
- Projection-based integration methodology
- Adaptive mesh refinement
- Parallel software infrastructure

Combining all of these elements resulted in several orders of magnitude improvement in performance.

Fundamental shift in the role of computing in the study of turbulent combustion

Issues for the future

Combustion

- For gaseous systems, simulation has caught up to experiment and model fidelity
 - Simulation of realistic flames with realistic models is now possible
 - Opportunity and need for closer ties between traditionally disparate activities
- Modeling of realistic systems
 - Liquid fuels
 - Complex moving geometry
 - Particulates
- Direct impact on design

Computational science challenges

- Tension between models, algorithms and machines
- Managing software complexity
- Extracting knowledge from data

As we move toward petascale machines, we should look at all aspects of how we compute